

Convergent Iterative Solutions of Schroedinger Equation for a Generalized Double Well Potential*

R. Friedberg¹, T. D. Lee^{1,2} and W. Q. Zhao^{2,3}

1. Physics Department, Columbia University, New York, NY 10027, USA

2. China Center of Advanced Science and Technology (CCAST)

(World Lab.), P.O. Box 8730, Beijing 100080, China

3. Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100039, China

February 1, 2008

Abstract

We present an explicit convergent iterative solution for the lowest energy state of the Schroedinger equation with a generalized double well potential $V = \frac{g^2}{2}(x^2 - 1)^2(x^2 + a)$. The condition for the convergence of the iteration procedure and the dependence of the shape of the groundstate wave function on the parameter a are discussed.

PACS: 11.10.Ef, 03.65.Ge

*Work supported in part by the U.S. Department of Energy

1. Introduction

This paper is stimulated by an interesting question raised by Roman Jackiw[1] concerning the extent of validity of the convergent iterative method[2-5] that we have developed for the N -dimensional generalization of the double well potential

$$V = \frac{g^2}{2}(r^2 - r_0^2)^2. \quad (1.1)$$

More specifically, whether the method is equally applicable to a different sombrero-shaped potential

$$V = \frac{g^2}{2}(r^2 - r_0^2)^2(r^2 + 2r_0^2). \quad (1.2)$$

The latter has several new features[1,6]. When $g^2 = 1$ and

$$r_0^4 = \frac{1}{3}(2 + N), \quad (1.3)$$

the groundstate wave function ψ is simply

$$e^{-r^4/4} \quad (1.4)$$

which peaks at $r = 0$. Yet for $g^2 \gg 1$, the maximum of ψ has to be near $r = r_0$. In particular, for a one-dimensional problem, as g^2 increases from 1, there would be a critical point when ψ changes from having a single maximum at the origin to one with double peaks. Thus, it is of interest to examine whether our convergent iterative method works for $g^2 = 1$ as well as for g^2 larger than 1. The purpose of this paper is to show that this is indeed the case.

To simplify our discussions, we examine only the one-dimensional case in this paper. Let $\psi(x)$ be the groundstate wave function of the Schroedinger equation

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E \psi(x) \quad (1.5)$$

with

$$V(x) = \frac{g^2}{2}(x^2 - 1)^2(x^2 + a) \quad (1.6)$$

and

$$a > 0. \quad (1.7)$$

We note that in one dimension, the potential (1.2)-(1.3) is a special case of (1.6) with $a = 2$. For convenience of nomenclature, in dimension > 1 we call (1.1) the sombrero potential, and (1.2) the generalized sombrero potential; in one dimension, we call

$$\frac{g^2}{2}(x^2 - 1)^2 \quad (1.8)$$

the double well potential and (1.6) the generalized double well potential.

In Section 2, we give a brief review of our convergent iterative method for the potential (1.6). To ensure rapid convergence, we have established a rather effective theorem, called Hierarchy Theorem, provided a certain inequality can be satisfied. This inequality is proved in Section 3 for $a = 2$ (i.e., the potential (1.2) in one-dimension), and in the Appendix for an arbitrary positive $a > a_c \cong 0.664$. Some of the pertinent numerical results are given in Section 4.

2. Trial Function and Iterative Equations

To construct a good trial function $\phi(x)$ for the groundstate wave function, we follow the same steps developed for the double-well potential[2-5]. The main components of $\phi(x)$ are constructed by using the Schroedinger equation (1.5) and extracting the first two terms of its perturbation series expansion of $\psi(x)$ and E in g^{-1} .

Write

$$\psi(x) = e^{-gS(x)} \quad (2.1)$$

and set

$$gS(x) = gS_0(x) + S_1(x) + g^{-1}S_2(x) + \dots \quad (2.2)$$

Correspondingly,

$$E = gE_0 + E_1 + g^{-1}E_2 + \dots \quad (2.3)$$

Substituting (2.1)-(2.3) into (1.5), we find

$$S'_0 = (x^2 - 1)\sqrt{x^2 + a}, \quad (2.4)$$

and

$$S_1' S_0' = \frac{1}{2} S_0'' - E_0. \quad (2.5)$$

Since the left side of (2.5) is zero at $x = 1$,

$$E_0 = \frac{1}{2} S_0''(1) = \sqrt{1+a}. \quad (2.6)$$

Thus,

$$S_1' = \frac{x(3x^2 + 2a - 1) - 2\sqrt{1+a}\sqrt{x^2+a}}{2(x^2-1)(x^2+a)}. \quad (2.7)$$

(Throughout the paper, prime denotes d/dx .) Next, introduce

$$\phi_+(x) \equiv \exp[-gS_0(x) - S_1(x)] \quad (2.8)$$

and

$$\phi_-(x) \equiv \exp[-gS_0(-x) - S_1(x)]. \quad (2.9)$$

We note that $\phi_+(x)$ and $\phi_-(x)$ are completely defined, except for a common arbitrary normalization factor. The trial function $\phi(x)$ is an even function of x , defined by

$$\phi(x) = \phi(-x) = \begin{cases} \phi_+(x) + \Gamma \phi_-(x) & \text{for } 0 \leq x < 1, \\ \{1 + [\Gamma \phi_-(1)/\phi_+(1)]\} \phi_+(x) & \text{for } x > 1, \end{cases} \quad (2.10)$$

with

$$\Gamma = -\frac{\phi_+'(0)}{\phi_-'(0)} = \frac{ga - \sqrt{1+a}}{ga + \sqrt{1+a}}. \quad (2.11)$$

In the following, we assume

$$g > \frac{1}{a} \sqrt{1+a}, \quad (2.12)$$

and therefore

$$\Gamma > 0. \quad (2.13)$$

By construction, $\phi'(0) = 0$. The functions $\phi(x)$ and $\phi'(x)$ are continuous everywhere. Since $\psi(x)$ and $\phi(x)$ are both even in x , we need only consider

$$x \geq 0 \quad (2.14)$$

in the following.

By differentiation, ϕ_+ and ϕ satisfy two Schroedinger equations

$$-\frac{1}{2}\phi_+'' + (V + u)\phi_+ = gE_0\phi_+ \quad (2.15)$$

and

$$-\frac{1}{2}\phi'' + (V + w)\phi = gE_0\phi, \quad (2.16)$$

where

$$u(x) = \frac{1}{2}(S_1'^2 - S_1'') \quad (2.17)$$

and

$$w(x) = u(x) + \hat{g}(x) \quad (2.18)$$

with

$$\hat{g}(x) = \begin{cases} gE_0 \frac{2\Gamma\phi_-}{(\phi_+ + \Gamma\phi_-)} & \text{for } 0 \leq x < 1 \\ 0 & \text{for } x > 1. \end{cases} \quad (2.19)$$

Thus, for

$$0 \leq x < 1, \quad (2.20)$$

$$\hat{g}'(x) = gE_0 \frac{2\Gamma\phi_+^2}{(\phi_+ + \Gamma\phi_-)^2} \left(\frac{\phi_-}{\phi_+} \right)'. \quad (2.21)$$

From (2.8)-(2.9), it follows that

$$\frac{\phi_-}{\phi_+} = e^{-2gS_0(0)} \cdot e^{2gS_0(x)}. \quad (2.22)$$

Within the range (2.20),

$$\left(\frac{\phi_-}{\phi_+} \right)' = \left(\frac{\phi_-}{\phi_+} \right) 2g(x^2 - 1)\sqrt{x^2 + a} < 0 \quad (2.23)$$

and therefore

$$\hat{g}'(x) < 0. \quad (2.24)$$

Thus, $\hat{g}(x)$ is a positive decreasing function of x . At $x = 1$, \hat{g} has a discontinuity, decreasing to zero for $x > 1$.

For the one-dimensional case of the generalized sombrero shaped potential (1.2)-(1.3), we have

$$N = 1, \quad r_0 = 1 \quad \text{and} \quad a = 2. \quad (2.25)$$

The corresponding potential is

$$V(x) = \frac{g^2}{2}(x^2 - 1)^2(x^2 + 2). \quad (2.26)$$

In the next section, it will be proved that for this potential, at all finite $x > 0$, we have

$$u(x) > 0 \quad (2.27)$$

and

$$u'(x) < 0. \quad (2.28)$$

Thus

$$w(x) > 0 \quad (2.29)$$

and

$$w'(x) < 0. \quad (2.30)$$

Furthermore, $w(\infty) = 0$. [The extension to the potential (1.6) with $a \neq 2$ will be discussed in the Appendix.]

Once the condition $w'(x) < 0$ is established, we can apply the Hierarchy Theorem[3,4], as we shall discuss.

Define

$$H_0 = -\frac{1}{2} \frac{d^2}{dx^2} + V(x) + w(x) \quad (2.31)$$

and write (2.16) as

$$(H_0 - gE_0)\phi(x) = 0. \quad (2.32)$$

The Schroedinger equation we would like to solve is (1.5), which can be written as

$$(H_0 - gE_0)\psi(x) = (w(x) - \mathcal{E})\psi(x) \quad (2.33)$$

where

$$\mathcal{E} = gE_0 - E. \quad (3.34)$$

Multiplying (2.33) by ϕ and (2.32) by ψ . Their difference gives

$$-\frac{1}{2}(\phi\psi' - \psi\phi')' = (w - \mathcal{E})\phi\psi. \quad (2.35)$$

Hence, the ratio

$$f = \psi/\phi \quad (2.36)$$

satisfies

$$-\frac{1}{2}(\phi^2 f')' = (w - \mathcal{E})\phi^2 f. \quad (2.37)$$

Its integral over all x gives

$$\mathcal{E} = \int_0^\infty w\phi^2 f \, dx / \int_0^\infty \phi^2 f \, dx. \quad (2.38)$$

Eqs. (2.37) and (2.38) can then be solved by considering the iterative series $\{f_n(x)\}$ and $\{\mathcal{E}_n\}$, with

$$-\frac{1}{2}(\phi^2 f'_n)' = (w - \mathcal{E}_n)\phi^2 f_{n-1} \quad (2.39)$$

and therefore

$$\mathcal{E}_n = \int_0^\infty w\phi^2 f_{n-1} dx / \int_0^\infty \phi^2 f_{n-1} dx. \quad (2.40)$$

We differentiate two different sets of boundary conditions:

$$(I) \quad f_n(\infty) = 1 \quad \text{for all } n \quad (2.41)$$

or

$$(II) \quad f_n(0) = 1 \quad \text{for all } n. \quad (2.42)$$

Thus, in case (I)

$$f_n(x) = 1 - 2 \int_x^\infty \frac{dy}{\phi^2(y)} \int_y^\infty (w(z) - \mathcal{E}_n)\phi^2(z) f_{n-1}(z) dz \quad (2.43)$$

and correspondingly in case (II)

$$f_n(x) = 1 - 2 \int_0^x \frac{dy}{\phi^2(y)} \int_0^y (w(z) - \mathcal{E}_n)\phi^2(z) f_{n-1}(z) dz. \quad (2.44)$$

In case (I), it can be readily verified that because $f_n(\infty) = 1$ and

$$f'_n < 0, \quad (2.45)$$

we have

$$f_n(0) > f_n(x) > f_n(\infty) = 1. \quad (2.46I)$$

In case (II), we assume $w(x)$ to be not too large so that (2.44) is consistent with

$$f_n(x) > 0 \text{ for all } x$$

and therefore

$$f_n(0) = 1 > f_n(x) > f_n(\infty) > 0. \quad (2.46\text{II})$$

As we shall see, these two boundary conditions (I) and (II) produce sequences that have very different behavior. Yet, they also share a number of common properties.

Now, assuming that $u'(x) < 0$ (section 3) and hence $w'(x) < 0$ (by (2.18) and (2.28)), we have from refs.[3,4]

Hierarchy Theorem. (I) With the boundary condition $f_n(\infty) = 1$, we have for all n

$$\mathcal{E}_{n+1} > \mathcal{E}_n \quad (2.47)$$

and

$$\frac{d}{dx} \left(\frac{f_{n+1}(x)}{f_n(x)} \right) < 0 \quad \text{at any } x > 0. \quad (2.48)$$

Thus, the sequences $\{\mathcal{E}_n\}$ and $\{f_n(x)\}$ are all monotonic, with

$$\mathcal{E}_1 < \mathcal{E}_2 < \mathcal{E}_3 < \dots \quad (2.49)$$

and

$$1 < f_1(x) < f_2(x) < f_3(x) < \dots \quad (2.50)$$

at all finite x .

(II) With the boundary condition $f_n(0) = 1$, we have for all odd $n = 2l + 1$ an ascending sequence

$$\mathcal{E}_1 < \mathcal{E}_3 < \mathcal{E}_5 < \dots, \quad (2.51)$$

but for all even $n = 2m$, a descending sequence

$$\mathcal{E}_2 > \mathcal{E}_4 > \mathcal{E}_6 > \dots. \quad (2.52)$$

Furthermore, between any even $n = 2m$ and any odd $n = 2l + 1$

$$\mathcal{E}_{2m} > \mathcal{E}_{2l+1}. \quad (2.53)$$

Likewise, at any x , for any even $n = 2m$

$$\frac{d}{dx} \left(\frac{f_{2m+1}(x)}{f_{2m}(x)} \right) < 0, \quad (2.54)$$

whereas for any odd $n = 2l + 1$

$$\frac{d}{dx} \left(\frac{f_{2l+2}(x)}{f_{2l+1}(x)} \right) > 0. \quad (2.55)$$

The groundstate energy E of the original Hamiltonian

$$H = -\frac{1}{2} \frac{d^2}{dx^2} + V(x) \quad (2.56)$$

is the limit of the sequence $\{E_n\}$ with

$$E_n = E_0 - \mathcal{E}_n. \quad (2.57)$$

Hence the boundary condition $f_n(\infty) = 1$ yields a sequence

$$E_1 > E_2 > E_3 > \cdots > E \quad (2.58)$$

with each member E_n an *upper* bound of E , similar to the usual variational method. On the other hand, with the boundary condition $f_n(0) = 1$, while the sequence of its odd members $n = 2l + 1$ yields a similar one, like (2.58) with

$$E_1 > E_3 > E_5 > \cdots > E, \quad (2.59)$$

its even members $n = 2m$ satisfy

$$E_2 < E_4 < E_6 < \cdots < E. \quad (2.60)$$

It is unusual to have an iterative sequence of lower bounds of the eigenvalue E . In both cases we have

$$\lim_{n \rightarrow \infty} E_n = E. \quad (2.61)$$

3. Proof of $u'(x) < 0$

In this section we shall establish $u'(x) < 0$ for the case $a = 2$ [i.e., the one-dimensional case of the generalized sombrero potential (1.2)]. The general case of arbitrary positive a will be discussed in the Appendix.

Write the potential $V(x)$ of (1.6) as

$$V(x) = g^2 v(x). \quad (3.1).$$

When $a = 2$,

$$v(x) = \frac{1}{2}(x^2 - 1)^2(x^2 + 2). \quad (3.2)$$

The functions $S_0(x)$ and $S_1(x)$ introduced in Section 2 are

$$S_0(x) = \frac{x}{4}(x^2 - 1)\sqrt{x^2 + 2} - \frac{3}{2}\ln(x + \sqrt{x^2 + 2}) \quad (3.3)$$

and

$$S_1(x) = \ln(x + 1) + \frac{1}{4}\ln(x^2 + 2) + \frac{1}{2}\ln \frac{2 + x + \sqrt{3(x^2 + 2)}}{2 - x + \sqrt{3(x^2 + 2)}}. \quad (3.4)$$

In accordance with (2.17), we find

$$u(x) = \frac{3}{8} \frac{25x^8 + 150x^6 + 393x^4 + 408x^2 + 144}{(x^2 + 2)^2(A + B)} \quad (3.5)$$

with

$$A = 5x^6 + 10x^4 + 21x^2 + 12 \quad (3.6)$$

and

$$B = 8\sqrt{3}x(x^2 + 1)\sqrt{x^2 + 2}. \quad (3.7)$$

Its derivative is

$$u'(x) = -\frac{3}{8} \frac{C_1\sqrt{x^2 + 2} + C_2}{\sqrt{x^2 + 2}(\alpha + \beta\sqrt{x^2 + 2})^2} \quad (3.8)$$

with

$$C_1 = 250x^{17} + 3000x^{15} + 16740x^{13} + 49880x^{11} + 83706x^9 + 77952x^7 \\ + 34008x^5 + 2880x^3 - 1152x, \quad (3.9)$$

$$C_2 = 8\sqrt{3}(322x^{12} + 2236x^{10} + 6322x^8 + 9672x^6 + 8904x^4 \\ + 4800x^2 + 1152), \quad (3.10)$$

$$\alpha = (x^2 + 2)^2 A \quad (3.11)$$

and

$$\beta = (x^2 + 2)^{\frac{3}{2}} B = 8\sqrt{3}x(x^2 + 1)(x^2 + 2)^2. \quad (3.12)$$

Because at all x

$$(4800x^2 + 1152)8\sqrt{3} > 1152x\sqrt{x^2 + 2}, \quad (3.13)$$

we have

$$C_1\sqrt{x^2 + 2} + C_2 > 0 \quad (3.14)$$

and therefore

$$u' < 0. \quad (3.15)$$

From (3.5), we see that $u > 0$ and therefore Hierarchy Theorem is applicable. The general case when $V(x)$ is given by (1.6) will be discussed in the Appendix. As we shall see, for $V(x) = g^2v(x)$,

$$v(x) = \frac{1}{2}(x^2 - 1)^2(x^2 + a) \quad (3.16)$$

and

$$a > a_c \cong 0.664, \quad (3.17)$$

the corresponding $u(x)$ also satisfies (3.15); i.e. $u'(x) < 0$ for all $x > 0$, and that ensures the applicability of the Hierarchy Theorem.

4. Numerical Results and Discussions

Throughout this section we denote the n^{th} order iterative solution as

$$\psi_n(x) = \psi_0(x)f_n(x) \quad (4.1)$$

with $f_n(x)$ the solution of (2.39) and $\psi_0(x)$ related to $\phi(x)$ of (2.10) by

$$\psi_0(x) = \phi(x)/\phi(0) \quad (4.2)$$

so that

$$\psi_0(0) = 1. \quad (4.3)$$

4.1 The case $a = 2$ and $g = 1$.

We first discuss the case of $a = 2$ and $g = 1$. The resultant series of energies are shown in Table 1. The energy series for two different boundary conditions converge in different ways.

I . For the boundary condition $f_n(\infty) = 1$ we find that the iterative energy sequence

$$E_0 > E_1 > E_2 > E_3 > \dots > E \quad (4.4)$$

is given numerically by

$$1.7321 > 1.0163 > 1.0031 > 1.0005 > 1.0001 > 1.0000 > \dots > E = 1. \quad (4.5)$$

II. For the boundary condition $f_n(0) = 1$, E_0 is still 1.7321, but the iterative energy sequence becomes

$$E_1 > E_3 > \dots > E > \dots > E_4 > E_2, \quad (4.6)$$

and is given numerically by

$$1.0163 > 1.0002 > \dots > E > \dots > 1.0000 > 0.9981. \quad (4.7)$$

To 4 decimal places E_4 is indistinguishable from the exact $E = 1$.

In both cases I and II, the zeroth order trial function $\psi_0(x)$ has a maximum near $x = 1$. However, to the accuracy of Figure 1, for $n = 2$ $\psi_2(x)$ is essentially the same as the exact groundstate wave function $\psi(x) = e^{-x^4/4}$. The

resultant series of wave functions and energies convergence rapidly to the exact expressions. It is interesting to notice that although the trial function has its two maxima near $x = \pm 1$, the iterative series gives the final wave function in the shape of the exact groundstate wave function with a single maximum at $x = 0$. The rapid change of the shape of the wave function from the trial one to the exact solution shows how the iteration procedure works.

4.2 The case $g = 1$.

Next we discuss the case of $g = 1$ for different values of a . The results of the energy series for the boundary condition II are given in Table 2.

As proved in Appendix, to ensure the convergence of the iterative series the parameter a should satisfy $a > a_c \cong 0.664$. We have chosen $g = 1$, $a = 3$, 2 and 1.8. The obtained wave functions are shown respectively in Figures 2, 1 and 3. The behavior of the final function for $a < 2$ is similar to the one at $a = 2$, namely the resultant wave function has only one maximum at $x = 0$, while the trial function has two maxima near $x = \pm 1$. When $a = 3$ the iterative wave function retains a similar shape as the trial function with its maxima at x near ± 1 , indicating that the exact groundstate wave function also has its maximum at x near ± 1 , like the trial function when $g = 1$ and $a = 3$.

4.3 The case $a = 2$.

Next we discuss the case $a = 2$ for different values of g . The results of the energy series for the boundary condition II are given in Table 3.

According to (2.12), for $a = 2$ the allowed values of g is $g > 0.866$. The wave functions for $a = 2$, $g = 3$, 1 and 0.88 are shown respectively in Figures 4, 1 and 5. The behavior of the final function for $g < 1$ is similar to the one at $g = 1$, namely the resultant wave function has only one maximum at $x = 0$, while the trial function has two maxima near $x = \pm 1$. When $g = 3$ the iterative wave function retains a similar shape as the trial function with its maxima at x near ± 1 , indicating that the exact groundstate wave function also has its maximum at x near ± 1 , like the trial function when $g = 3$ and $a = 2$.

Table 1. Eigenvalues of groundstates for $g = 1$ and $a = 2$

	E_0	E_1	E_2	E_3	E_4	E_5
I	1.7321	1.0163	1.0031	1.0005	1.0001	1.0000
II	1.7321	1.0163	0.9981	1.0002	1.0000	1.0000

**Table 2. Eigenvalues of groundstates for $g = 1$,
using II with $f_n(0) = 1$ as the boundary condition**

a	E_0	E_1	E_2	E_3	E_4	E_5
1.8	1.6733	0.9558	0.9418	0.9432	0.9431	0.9431
2	1.7321	1.0163	0.9981	1.0002	1.0000	1.0000
3	2.0000	1.2974	1.2602	1.2659	1.2651	1.2652

**Table 3. Eigenvalues of groundstates for $a = 2$
using II with $f_n(0) = 1$ as the boundary condition**

g	E_0	E_1	E_2	E_3	E_4	E_5
0.88	1.5242	0.8633	0.8517	0.8528	0.8527	0.8527
1	1.7321	1.0163	0.9981	1.0002	1.0000	1.0000
2	3.4641	2.6934	2.6375	2.6465	2.6455	2.6456
3	5.1962	4.5786	4.5562	4.5591	4.5589	4.5589

References

- [1] R. Jackiw, Private communications.
- [2] R. Friedberg, T. D. Lee, W. Q. Zhao and A. Cimenser
Ann. Phys. 294 (2001), 67
- [3] R. Friedberg and T. D. Lee, Ann. Phys. 308 (2003), 263
- [4] R. Friedberg and T. D. Lee, Ann. Phys. 316(2005), 44
- [5] R. Friedberg, T. D. Lee and W. Q. Zhao, Ann. Phys. 321 (2006), 1981
- [6] G. 't Hooft and S. Nobbenhuis, Class. Quant. Grav. 23(2006), 3819

Appendix

In this Appendix we give the proof of the convergence of the iterative series for the generalized double-well potential, eq.(1.6)

$$V(x) = g^2 v(x) \quad \text{and} \quad v(x) = \frac{1}{2}(x^2 - 1)^2(x^2 + a), \quad (A.1)$$

where a is an arbitrary constant.

Following the steps described in Section 2, from (2.4), (2.7) and (2.17) we have

$$u(x) = \frac{\alpha - 8\sqrt{x^2 + a} \beta}{8(x^2 - 1)^2(x^2 + a)^2} \quad (A.2)$$

where

$$\alpha = 15x^6 + 6(3a - 1)x^4 + (8a^2 + 12a + 7)x^2 + 8a^2 + 2a \quad (A.3)$$

and

$$\beta = \sqrt{1 + a} x(3x^2 + 2a - 1). \quad (A.4)$$

Integrating (2.4) and (2.7) gives

$$\begin{aligned} S_0(x) = & \frac{1}{4}x(\sqrt{x^2 + a})^3 - \left(\frac{a}{8} + \frac{1}{2}\right)x\sqrt{x^2 + a} \\ & - a\left(\frac{a}{8} + \frac{1}{2}\right)\ln(x + \sqrt{x^2 + a}) \end{aligned} \quad (A.5)$$

and

$$S_1(x) = \ln(x + 1)(x^2 + a)^{1/4} + \frac{1}{2} \ln \frac{\sqrt{a + 1}\sqrt{x^2 + a} + a + x}{\sqrt{a + 1}\sqrt{x^2 + a} + a - x}. \quad (A.6)$$

The corresponding trial function (2.10) satisfies the Schroedinger equation (2.16) with $w(x)$ expressed by (2.18) and (2.19).

According to the Hierarchy Theorem proved in Ref.[3,4] the iterative series is convergent if the potential $w(x)$, defined by (2.18), satisfies the conditions $w(x) > 0$ and $w'(x) < 0$. As we shall prove, when

$$a > a_c \cong 0.664, \quad (A.7)$$

the potential $u(x)$, defined by (2.17), satisfies $u(x) > 0$ and $u'(x) < 0$. Furthermore, when g satisfies (2.12), i.e.

$$a > a_g = \frac{1 + \sqrt{1 + 4g^2}}{2g^2} \quad (A.8)$$

we have $\Gamma > 0$ from (2.13); therefore $\hat{g}(x) > 0$ and $\hat{g}'(x) < 0$. Combining these results we have

$$w(x) > 0 \text{ and } w'(x) < 0 \quad \text{when } a > a_m = \max(a_c, a_g). \quad (A.9)$$

This condition ensures the convergent iterative solution for the groundstate of the generalized double-well potential (A.1) (i.e. (1.6)), in accordance with the Hierarchy theorem.

Range of parameter a

As mentioned above, to obtain a convergent iterative series the potential $u(x)$ in (A.2) should satisfy

$$u(x) > 0 \quad \text{and} \quad u'(x) < 0. \quad (A.10)$$

For $a > 0$, introducing

$$\gamma_{\pm} \equiv \alpha \pm 8\sqrt{x^2 + a} \beta \quad (A.11)$$

with α and β given by (A.3)-(A.4), we have

$$\gamma_+ \gamma_- \equiv (x^2 - 1)^2 \gamma = \alpha^2 - 64(x^2 + a) \beta^2. \quad (A.12)$$

Thus, $u(x)$ can be expressed as

$$u = \frac{\gamma_-}{8(x^2 + a)^2(x^2 - 1)^2} \quad (A.13)$$

and

$$u = \frac{1}{8(x^2 + a)^2} \left(\frac{\gamma}{\gamma_+} \right). \quad (A.14)$$

Write

$$\gamma = \gamma(a, x) = g_1(x)(15x^4 + 36ax^2) + g_2 \quad (A.15)$$

where

$$g_1(x) = 15x^4 + 18x^2 - 1 \quad (A.16)$$

and

$$g_2 = g_2(a, x^2) = 4(141x^4 + 90x^2 + 1)a^2 + 32(9x^2 + 1)a^3 + 64a^4 > 0. \quad (A.17)$$

Consider only the first quadrant in (x, a) -plane with x, a positive. Define x_0 to be the point satisfying $g_1(x_0) = 0$. For $x > x_0$, $g_1(x) > 0$ and therefore, $\gamma > 0$. For $x < x_0$, $g_1(x) < 0$ and

$$\frac{\partial}{\partial a} \left(\frac{\gamma}{a^2} \right) > 0 \quad \text{for } a > 0. \quad (A.18)$$

Since $(\gamma/a^2) \rightarrow -\infty$ when $a \rightarrow 0$ and $(\gamma/a^2) \rightarrow \infty$ when $a \rightarrow \infty$, at a fixed $x < x_0$ by varying the parameter a from 0 to ∞ , $\gamma(a, x) = 0$ only once. We define a curve (G) in x , satisfying $\gamma(a, x) = 0$ and a curve (B) satisfying $\beta(a, x) = 0$ as shown in Fig. A1. It can be seen that above the curves (B) and (G) , β and γ are both positive. The curve (B) is above the curve (G) . Therefore above the curves (B) γ_+ , γ and u are all positive. Below the curve (B) β is negative; therefore γ_- and u are positive. Thus we can conclude that $u(x) > 0$ everywhere for $a > 0$.

By differentiating u , we have

$$\left(\frac{\partial u}{\partial x} \right)_a = u'(x) \equiv \frac{\tilde{\gamma}_-}{8(x^2 + a)^3(x^2 - 1)^3}, \quad (A.19)$$

where

$$\tilde{\gamma}_- = \tilde{\alpha} - 8\sqrt{x^2 + a} \tilde{\beta} \quad (A.20)$$

with

$$\begin{aligned} \tilde{\alpha} &= [x^4 + (a - 1)x^2 - a]\alpha' - [8x^3 + 4(a - 1)x]\alpha \\ &= (-30x^9 - 6x^7 - 42x^5 + 14x^3) + (-42x^7 - 162x^5 + 18x^3 - 6x)a \\ &\quad + (-48x^5 - 144x^3)a^2 + (-16x^3 - 48x)a^3 \end{aligned} \quad (A.21)$$

and

$$\begin{aligned} \tilde{\beta} &= (x^2 + a)(x^2 - 1)\beta' - [7x^3 + (4a - 3)x]\beta \\ &= \sqrt{a + 1} \left[(-12x^6 + 6x^4 - 2x^2) + (-15x^4 - 2x^2 + 1)a + (-6x^2 - 2)a^2 \right]. \end{aligned} \quad (A.22)$$

Defining

$$\tilde{\gamma}_{\pm} \equiv \tilde{\alpha} \pm 8\sqrt{x^2 + a} \tilde{\beta} \quad (A.23)$$

we have

$$\begin{aligned}\tilde{\gamma}_+\tilde{\gamma}_- &= (x^2 - 1)^3\tilde{\gamma} \\ &= \tilde{\alpha}^2 - 64(x^2 + a)\tilde{\beta}^2.\end{aligned}\tag{A.24}$$

Therefore

$$u' = \frac{1}{8(x^2 + a)^3} \left(\frac{\tilde{\gamma}}{\tilde{\gamma}_+} \right).\tag{A.25}$$

It is straightforward to show after some derivation that $\tilde{\gamma}$ is a polynomial of x^2 and a . Defining

$$\tilde{\gamma} \equiv \sum_{\lambda=0}^6 \tilde{\Gamma}_\lambda x^{2\lambda}\tag{A.26}$$

where $\tilde{\Gamma}_\lambda$ are polynomials of a :

$$\begin{aligned}\tilde{\Gamma}_0 &= a^3[64 - 192a + 256a^3] \\ \tilde{\Gamma}_1 &= a^2[-228 - 1152a^2 + 1536a^3] \\ \tilde{\Gamma}_2 &= a[168 + 1068a - 960a^2 + 3648a^3] \\ \tilde{\Gamma}_3 &= 60 - 504a + 4500a^2 + 4992a^3 \\ \tilde{\Gamma}_4 &= -180 + 8568a + 4644a^2 \\ \tilde{\Gamma}_5 &= 3060 + 2520a \\ \tilde{\Gamma}_6 &= 900.\end{aligned}\tag{A.27}$$

For small a , it is convenient to introduce

$$z \equiv x^2/a, \quad \text{i.e.} \quad x^2 = az.\tag{A.28}$$

We can plot three curves on the (z, a) -plane : the curve (\tilde{A}) : $\tilde{\alpha} = 0$, (\tilde{B}) : $\tilde{\beta} = 0$ and (\tilde{G}) : $\tilde{\gamma} = 0$. The regions above the three curves correspond to $\tilde{\alpha} < 0$, $\tilde{\beta} < 0$ and $\tilde{\gamma} > 0$, respectively (see Fig. A2 for details). Above the critical point C , i.e. $a > a_c \cong 0.664$ we have $u' < 0$ from (A.23) and (A.25). Therefore this is the condition for $u > 0$ and $u' < 0$.

Figure Caption

Fig. 1 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 1$ and $a = 2$.

Fig. 2 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 1$ and $a = 3$.

Fig. 3 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 1$ and $a = 1.8$.

Fig. 4 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 3$ and $a = 2$.

Fig. 5 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 0.88$ and $a = 2$.

Fig. A1 Curves for $\beta = 0$ and $\gamma = 0$.

Fig. A2 Curves for $\tilde{\alpha} = 0$, $\tilde{\beta} = 0$ and $\tilde{\gamma} = 0$.

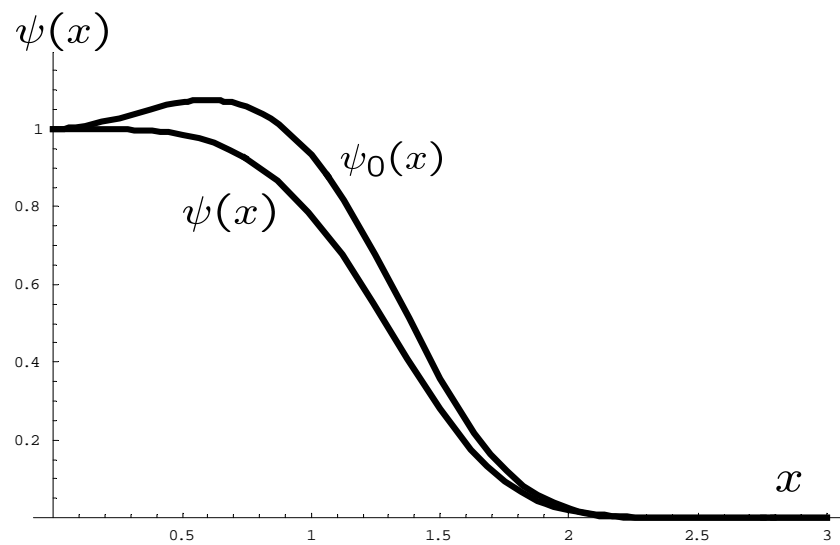


Fig. 1 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 1$ and $a = 2$.

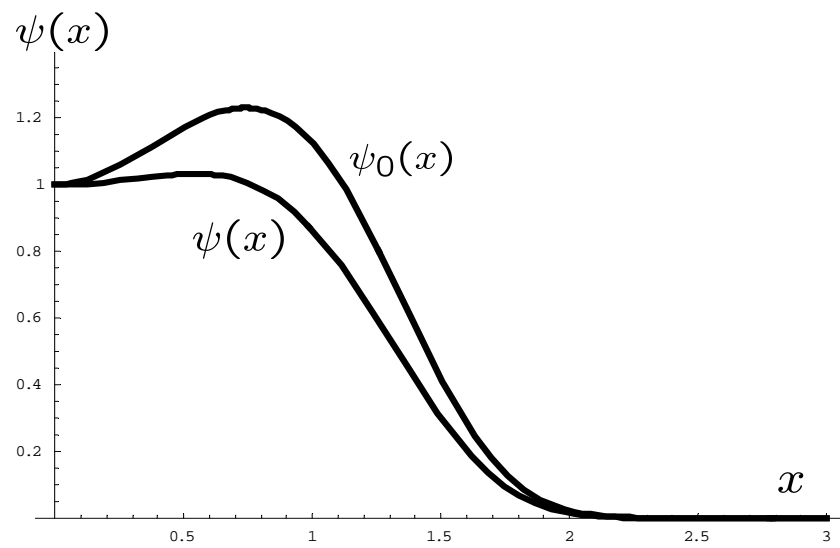


Fig. 2 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 1$ and $a = 3$.

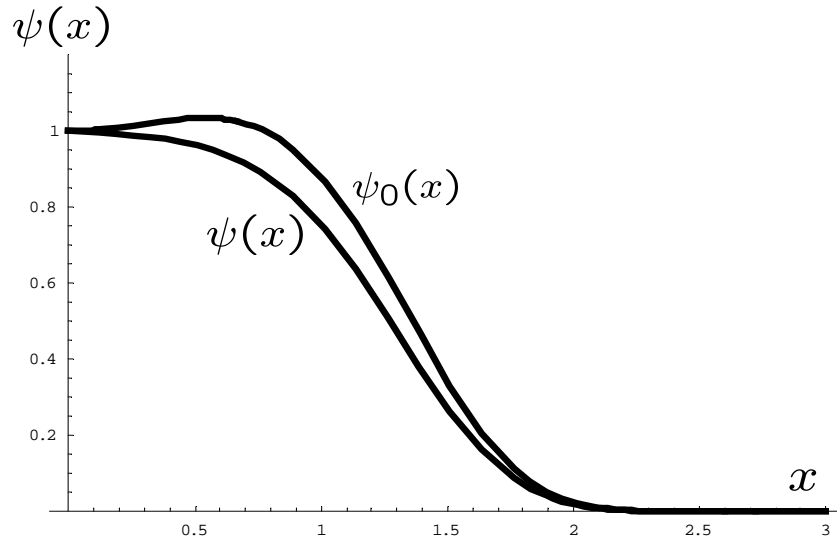


Fig. 3 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 1$ and $a = 1.8$.

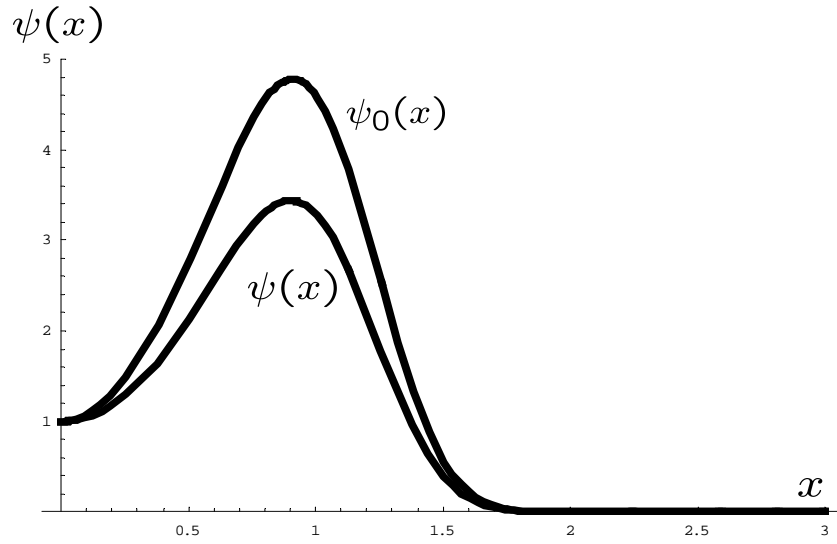


Fig. 4 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 3$ and $a = 2$.

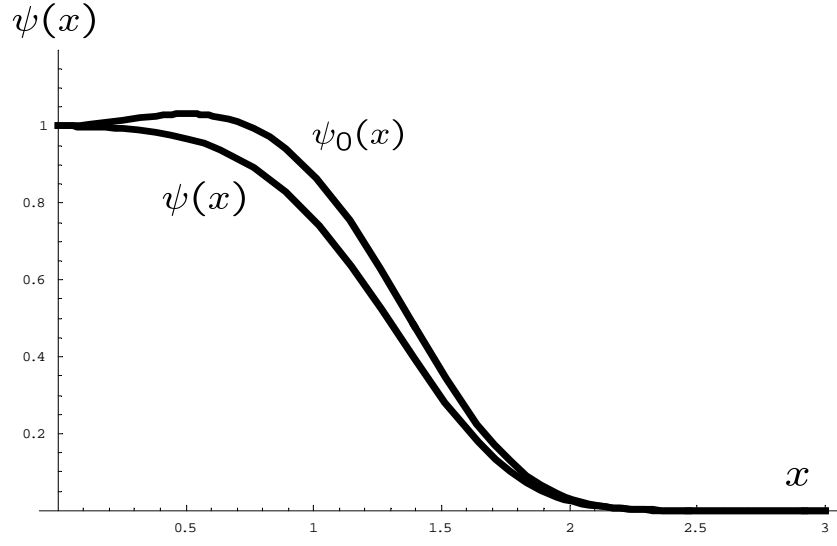


Fig. 5 Trial Function $\psi_0(x)$ and Groundstate Wave Function $\psi(x)$ for $g = 0.88$ and $a = 2$.

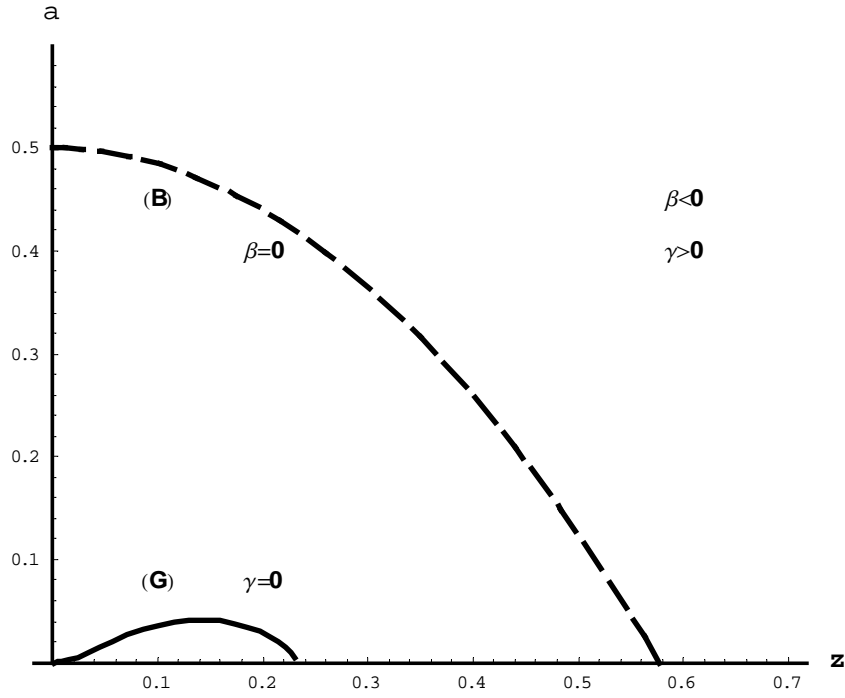


Fig. A1 Curves for $\beta = 0$ and $\gamma = 0$.

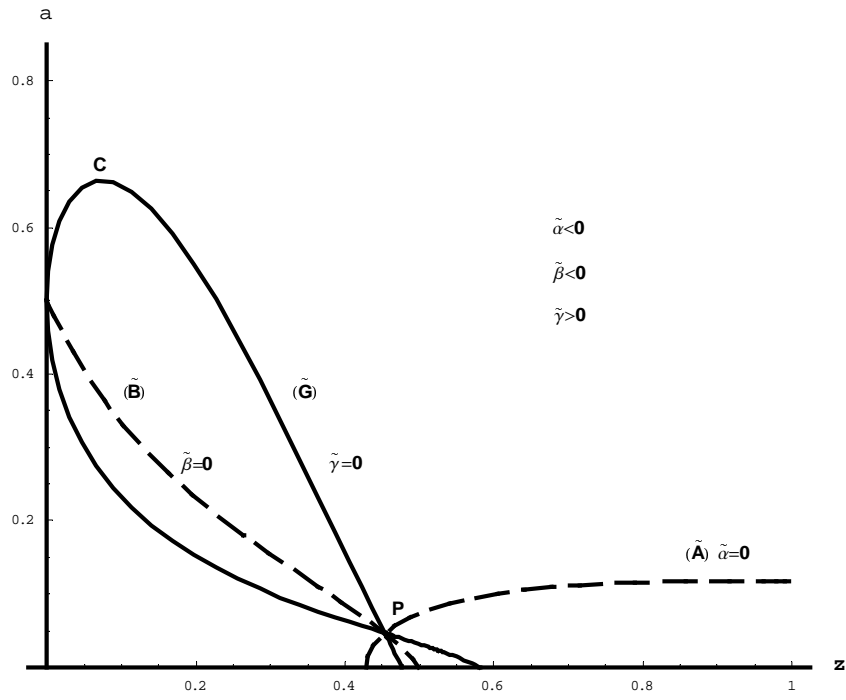


Fig. A2 Curves for $\tilde{\alpha} = 0$, $\tilde{\beta} = 0$ and $\tilde{\gamma} = 0$.